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QUANTUM CHEMICAL STUDY OF N-SUBSTITUTED ARYLAMINES AS ANALYTICAL REAGENTS

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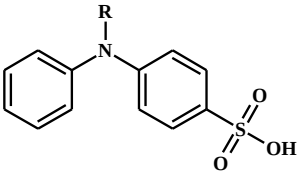
The great practical importance of arylmines in various fields of chemistry and chemical technology is the reason for interest to the study of their properties. It should be noted the role of arylamines in the theory evolution of the quantitative structure-property relationships. Although examples of the analytical systems selection based on the structure-property relationship are known, most of the new techniques are developed on the basis of the initial application, and the simulation are used mainly to explain the obtained data.

The theoretical study a number of sulfo-derivatives of N-substituted arylamines to predict their behavior in reduction–oxidation reaction was performed at the present work.



Реагент	R
DPASA	H
MDPASA	CH_3
DPASA	C_2H_5
TPASA	C_6H_5

The calculations of arylamine, their protonated state and cation-radicals were performed in the software package FireFly 8.0. A search of the equilibrium geometry was carried out using MP2/6-31G(d,p)/RHF/6-31G(d) and B3LYP/6-31G(d,p). Analytical vibrational frequency computations at the optimized structure were then performed to confirm that the optimized structure was at an energy minimum. Visualization of the structures and HOMO and LUMO molecular orbitals was performed with ChemCraft (1.7). Conformational analysis of arylamines was performed by Monte-Carlo method in Hyperchem (1.7).

The steric effect of N-substituents on the structural, electronic properties and conformational behavior of arylamine was estimated. The reduction potential, acid-base properties, spectral characteristics and behavior of arylamines in catalityc and enzyme reduction–oxidation reactions were predicted and confirmed experimentally.

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